

Chemical bond - quantum effect.

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Quantum mechanics is the science that describes our reality. More precisely, quantum mechanics describes our microcosm: the world of molecules, atoms, nuclei and elementary particles. That is, without quantum mechanics, we would not be able to correctly describe reality, as well as create modern electronic devices.

The world of quantum mechanics is described by the laws of nature, which are fundamentally different from the laws of the macrocosm in which we exist. Therefore, if we use classical physics (classical mechanics, thermodynamics, statistical physics and classical electrodynamics) to describe the microworld, then it is impossible to rationally explain and describe our reality. Misunderstanding of quantum mechanics is a consequence of the fact that people are trying to apply laws that, by definition, cannot describe the microcosm.

For example, Bohr in his doctoral dissertation (1911) on the classical electronic theory of metals proved a theorem according to which the magnetic moment of any set of elementary electric charges moving according to the laws of classical mechanics in a constant magnetic field is equal to zero in a stationary state.

“...In 1919, this theorem was independently rediscovered by Hendrik van Leeuwen and is called the Bohr-van Leeuwen theorem. It directly follows from it that it is impossible to explain the magnetic properties of matter (in particular, diamagnetism), while remaining within the framework of classical physics. This, apparently, was the first Bohr's collision with the limitations of the classical description, which led him to questions of quantum theory...” [1].

That is, if we want to correctly describe the real magnetic properties of substances, we need to abandon the classical laws.

Similarly, with electromagnetic radiation - for a correct description of the ultraviolet catastrophe we just need to accept that radiation represents certain portions of energy (quanta, 1901, M. Planck). Recall that the classical description considers electromagnetic radiation as an infinitely long wave.

The world of molecules (on the order of several angstroms) is also described by quantum mechanics. That is why the chemical bond is a purely quantum effect, which we will strictly show below. Consequently, the representation of a chemical bond as an electromagnetic interaction of nuclei and moving electrons is fundamentally wrong (this is a typically classical approach). Naturally, such a description will not be successful, and as a result, there is no physical justification, no predictive power, but only highly simplified, approximate and non-rigorous calculation methods. So, let's proceed to the proof that the chemical bond is a purely quantum effect.

Recall that quantum effects begin to manifest themselves significantly when the distance between interacting particles becomes smaller than the de Broglie wave.

$$\lambda = h / (m * v)$$

Since particles in the microcosm are in constant specific motion, then, according to de Broglie, each such particle will correspond to a wave of a certain length. If the particles are inside such a wave, then the interaction between them will be of a quantum mechanical nature, that is, it will be quantum. The laws of classical physics no longer play a decisive role.

From here, the mechanism of formation of a chemical bond strictly follows: for the formation of a bond, it is necessary that the nuclei of atoms be inside the de Broglie waves of valence electrons, only under this condition is quantum mechanical interaction between atoms possible. Further, we will show that the distance between chemically bound nuclei is always and in all types of bonding less than the de Broglie waves of valence electrons. This is irrefutable proof that the chemical bond is a quantum mechanical effect. So let's get to the proof.

Using Bohr's principle of complementarity, we can legitimately consider the valence electrons of an atom and the electrons of a chemical bond as point particles that move at a certain speed. For example, in a Bohr hydrogen atom, an electron moves along an orbit of radius $r = 0.5292 \text{ \AA}$, with a speed $v = 2.1877 * 10^6 \text{ m/s}$. Then, the length of the standing wave in the Bohr orbit will be equal to:

$$\lambda = 2 * \pi * r = 3.3249 \text{ \AA}$$

Given that the chemical bond is formed by the valence electrons of the atom, and knowing the length of the de Broglie wave of the valence electron, we can easily determine the length of the chemical bond.

Here it is necessary to clarify that the chemical bond can be represented as the vibrations of a string. Moreover, in our consideration, the string will be a standing de Broglie wave between the nuclei. The nuclei of atoms are the nodes of a standing wave. Such a representation follows from the fact that the vibrations of an ordinary string are determined by the linear density of the string and the force of the string tension. The chemical bond also has a certain linear density (energy), which is strictly correlated with the bond multiplicity. In addition, the linear density of a chemical bond from a physical point of view can be interpreted as a force that holds the nuclei of atoms ($F = E / L$). Below is a quote.

“...Therefore, based on the multiplicity of the chemical bond, more precisely, from the linear density (bond), it can be argued that the chemical bond is a standing wave with a certain linear density. Thus, a chemical bond can be considered as an oscillating string with a certain frequency (standing wave). It is clear that this vibration frequency will determine the energy of a given chemical bond. That is, a chemical bond is

a certain quantum of energy, since the standing waves of the string are perfectly quantized. Naturally, the de Broglie wave of the electron will form a standing wave...” [2].

Since the standing wave of the string is quantized, an integer number of half-waves ($\lambda/2$) will fit along the length of the string:

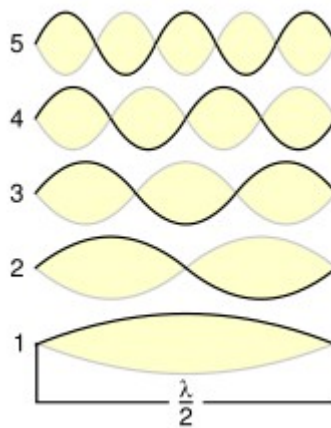
$$L = (\lambda / 2) * n$$

where L is the length of the chemical bond (the distance between the nuclei of atoms),

λ is the de Broglie wavelength of the valence electron,

$n = 1, 2, 3 \dots$

Look at the picture that shows the vibrations of a string attached to the ends [3].



In the ground state ($n = 1$), the standing wave of the string will be an ordinary chemical bond. Then, the length of the chemical bond will be equal to the de Broglie half-wave length ($\lambda/2$).

$$L = \lambda / 2$$

Given that the de Broglie wavelength in the Bohr orbit is 3.3249 \AA ($\approx 3.33 \text{ \AA}$), we can easily obtain the theoretical length of a chemical bond that a hydrogen atom can form.

$$L = \lambda / 2 = 3.3249 \text{ \AA} / 2 = 1.6625 \text{ \AA} \approx 1.66 \text{ \AA}.$$

But, since during the transition of a valence electron from the Bohr orbit to a chemical bond, additional energy is released, due to taking into account the “longitudinal mass” [4], the length of a real chemical bond will always be less than the theoretical value calculated by us (than more energy, the shorter the wavelength). For example, in a molecular hydrogen ion and in a hydrogen molecule, the length of a chemical bond formed from one and, respectively, two valence electrons is:

$$L(H_2^+) = 1.06 \text{ \AA}$$

$$L(H-H) = 0.7416 \text{ \AA}$$

That is, the length of both bonds is less than 1.66 Å, which was to be expected based on our assumptions.

In fact, the “maximum” bond length obtained by us for the Bohr electron of hydrogen (1.66 Å) limits the length of “strong” chemical bonds in which a hydrogen atom can participate.

But, since the length of the de Broglie wave for a hydrogen electron is 3.33 Å, then “weak” chemical bonds involving a hydrogen atom can have a length of up to 3.33 Å. Theoretically, an even greater increase in the bond length, that is, more than 3.33 Å, is possible due to a change in the characteristics of the valence electron, and, consequently, an increase in the length of the de Broglie wave. But, such an increase will lead to a very strong decrease in the binding energy - these will already be “ultra-weak” bonds with the participation of a hydrogen atom.

The above is confirmed by real hydrogen bonds, which are divided into “weak” (energy of the order of 20 - 50 kJ/mol) and “strong” hydrogen bonds with an energy of 100 kJ/mol or more. Moreover, the length of “weak” hydrogen bonds is indeed more than 1.66 Å (up to 3 Å and more), and the length of “strong” bonds is less than 1.66 Å (hydrogen and ordinary covalent bonds involving a hydrogen atom).

It is also commonly believed that atoms can be linked by a hydrogen bond if the distance between them is up to 3.6 Å, which fully confirms what has been said.

Let us clarify that when calculating the bond length, another atom must also be taken into account, because valence electrons of different atoms participate in the classical covalent two-electron bond. Therefore, for a more accurate analysis of bonds involving hydrogen, we calculate the length of the de Broglie wave of the valence electron for oxygen and fluorine atoms.

For calculations, we assume that the valence electron rotates in a circular “Bohr” orbit of the corresponding atom. Then, the real radius of the atom will be the “Bohr” radius for a particular atom. In this case, the calculations are completely similar to those given above.

The radius of the oxygen atom, according to Enrico Clementi is 0.48 Å [5].

Calculate the wavelength and half-wave.

$$r(O) = 0.48 \text{ \AA}$$

$$\lambda = 2 * \pi * r = 3.0159 \text{ \AA} \approx 3 \text{ \AA}$$

$$L = \lambda / 2 = 3.0159 \text{ \AA} / 2 = 1.5080 \text{ \AA} \approx 1.5 \text{ \AA}.$$

According to the calculation, “strong” bonds involving hydrogen and oxygen atoms will be less than 1.5 Å, and “weak” bonds will be more than 1.5 Å, but less than 3 Å. Then, “ultra-weak” bonds (OH) will have a length of more than 3 Å.

The radius of the fluorine atom according to Clementi is 0.42 Å [5]. Calculate the wavelength and half-wave.

$$r(\text{F}) = 0.42 \text{ Å}$$

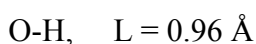
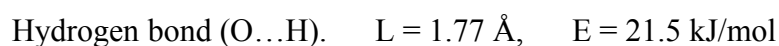
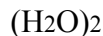
$$\lambda = 2 * \pi * r = 2.6389 \text{ Å} \approx 2.64 \text{ Å}$$

$$L = \lambda / 2 = 2.6389 \text{ Å} / 2 = 1.3195 \text{ Å} \approx 1.32 \text{ Å}.$$

That is, “strong” bonds involving hydrogen and fluorine atoms will be less than 1.32 Å, and “weak” bonds will be more than 1.32 Å, but less than 2.64 Å.

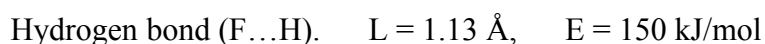
To confirm the results obtained, we consider the energy and length of bonds involving hydrogen in the water dimer, in the difluoride anion, and in hydrogen fluoride [6].

In the water dimer (H₂O)₂, the hydrogen bond length is 1.77 Å and the energy is 21.5 kJ/mol. The length of an ordinary O-H covalent bond is 0.96 Å.



That is, in the water dimer, the “weak” hydrogen bond has a length of more than 1.5 Å, as we predicted (greater than the half-wave length of oxygen and hydrogen atoms, 1.5 Å, 1.66 Å). And the usual covalent O-H bond has a length less than the indicated values.

In the difluoride anion [F...H...F][−] both hydrogen bonds are equal. The length of one such bond is 1.13 Å, and the energy is 150 kJ/mol.



As you can see, the “strong” hydrogen bond in the difluoride anion has a length of 1.13 Å, that is, less than the half-wave length of the fluorine atom (1.32 Å), and naturally less than the hydrogen half-wave (1.66 Å). This is indeed a “strong” hydrogen bond, since its energy is 150 kJ/mol.

The usual H-F covalent bond in hydrogen fluoride has a length of 0.92 Å, which is also less than the half-wave of the fluorine atom (1.32 Å).

$$\text{H-F}, \quad L = 0.92 \text{ Å}$$

It is interesting to note that the single bond in the fluorine molecule has a length of 1.404 Å, which is slightly longer than the half-wavelength of the valence electron for the fluorine atom (1.32 Å).

$$L(\text{F-F}) = 1.404 \text{ Å}$$

$$\lambda / 2 = 1.32 \text{ Å}$$

Such an increase in the length of a chemical bond is due to the repulsion of electron pairs of different fluorine atoms (each atom has three pairs). Therefore, it can be strictly stated that the multiplicity of bond in a fluorine molecule will be less than unity.

Next, we will analyze the carbon atom, since the chemistry of carbon is the basis of our life.

The radius of the carbon atom according to Clementi is 0.67 Å [5]. Calculate the wavelength and half-wave for the valence electron.

$$r(\text{C}) = 0.67 \text{ Å}$$

$$\lambda = 2 * \pi * r = 4.2097 \text{ Å} \approx 4.21 \text{ Å}$$

$$L = \lambda / 2 = 4.2097 \text{ Å} / 2 = 2.1049 \text{ Å} \approx 2.11 \text{ Å}.$$

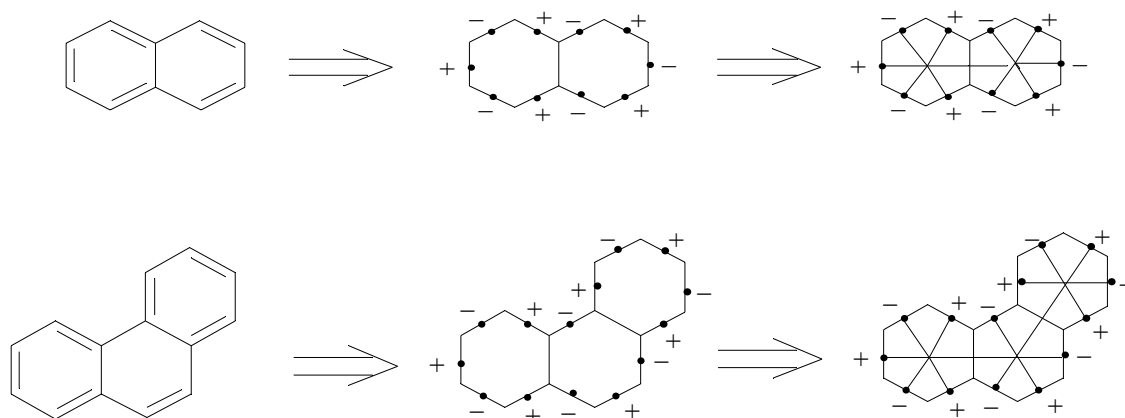
Therefore, “strong” C-C bonds will have a length of less than 2.11 Å, and “weak” C-C bonds will be greater than 2.11 Å, but less than 4.21 Å. “Ultra-weak” C-C bonds will have a length greater than 4.21 Å.

This is true. Here are the data on the length and energy of C-C bonds in ethane, ethylene and acetylene [7].

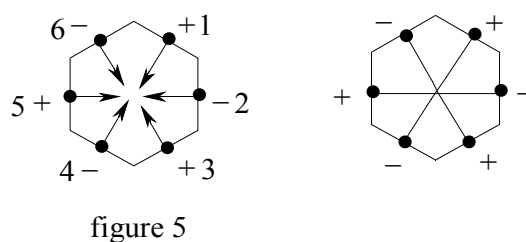
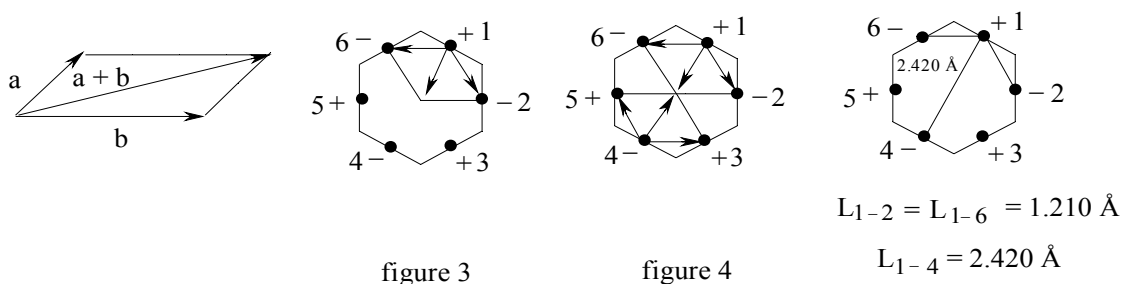
$\text{H}_3\text{C}-\text{CH}_3$	$\text{H}_2\text{C}=\text{CH}_2$	$\text{HC}\equiv\text{CH}$
$L_{\text{C}-\text{C}} = 1.543 \text{ Å}$	$L_{\text{C}=\text{C}} = 1.338 \text{ Å}$	$L_{\text{C}\equiv\text{C}} = 1.205 \text{ Å}$
$\text{H}_3\text{C}-\text{CH}_3$	$\text{H}_2\text{C}=\text{CH}_2$	$\text{HC}\equiv\text{CH}$
$E_{\text{C}-\text{C}} = 347.9397 \text{ kJ/mole}$	$E_{\text{C}=\text{C}} = 615.489 \text{ kJ/mole}$	$E_{\text{C}\equiv\text{C}} = 812.278 \text{ kJ/mole}$

It is clear that these covalent bonds are “strong” bonds.

Another thing is interesting, in benzene and other aromatic compounds there are also “weak” C-C bonds - this is an interaction through a cycle. This type of interaction in condensed aromatic compounds such as naphthalene, anthracene, phenanthrene, coronene, benzpyrene, etc. are typical “weak” and “ultra-weak” C-C bonds. Here is the molecular structure of naphthalene and phenanthrene [8]:



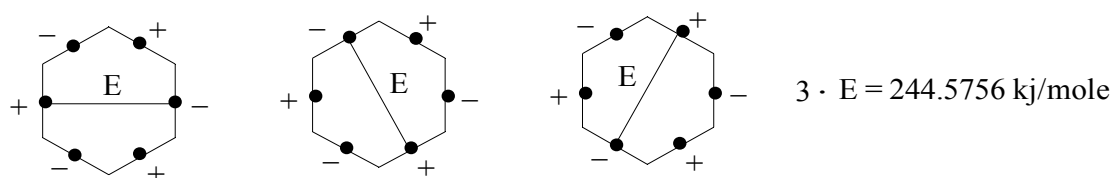
In benzene, the interaction through the cycle is formally a “weak” C-C bond, but in energy it is very close to “strong” chemical bonds: the length of such a bond is 2.42 Å, and the energy is 81.5252 kJ/mol. In fact, a bond with an energy greater than 80 kJ/mol can be considered a “strong” bond - it's just a matter of classification [8, p. 4-5].



$$L(1-4, 2-5, 3-6) = 2.42 \text{ Å}$$

As we can see from the scheme of the benzene molecule, when interacting through the cycle, the electrons (or three-electron bonds) are at a distance of 2.42 Å, which is more than the half-wavelength for the valence electron of carbon (2.11 Å), but less than the wavelength (4.21 Å). The energy of one such interaction is 81.5252 kJ/mol [8, p. 10-11].

The three interactions through the cycle represent the delocalization energy of benzene [8, p. 11]:



The interaction between graphite layers is also a typical “weak” chemical bond: the distance between the layers is 3.35 Å, which is greater than the half-wavelength (2.11 Å), but less than the wavelength (4.21 Å) of the carbon valence electron.

This approach to the explanation of the chemical bond easily describes the metallic bond. Consider alkali metals.

Recall that a metallic bond becomes covalent upon evaporation of alkali metals - metal vapors consist of diatomic Me-Me molecules and free atoms (during the condensation of vapors, we again obtain a metallic bond). The energy and length of the Me-Me covalent bond in the corresponding dimers are shown [9]:

Li ₂ ,	L(Li-Li) = 2.67 Å,	E(Li-Li) = 102 kJ/mol
Na ₂ ,	L(Na-Na) = 3.08 Å,	E(Na-Na) = 73 kJ/mol
K ₂ ,	L(K-K) = 3.92 Å,	E(K-K) = 57 kJ/mol
Rb ₂ ,	L(Rb-Rb) = 4.10 Å,	E(Rb-Rb) = 49 kJ/mol
Cs ₂ ,	L(Cs-Cs) = 4.30 Å,	E(Cs-Cs) = 42 kJ/mol

That is, a single bond in Me-Me diatomic alkali metal molecules is a typical covalent bond, the energy of which is slightly underestimated due to the large bond length, which is absolutely normal, since the energy and chemical bond length are strictly correlated (the longer the length, the less energy).

We especially note that in metals (metal bond), the nuclei of atoms are located at a distance that is much greater than the corresponding Me-Me single bond. For example, the translational lattice constant of a

lithium crystal is $a = 3.502 \text{ \AA}$, and the Li-Li covalent bond length in a dimer is 2.67 \AA . Similarly for other metals [9].

$$\text{Li} \rightarrow \quad a = 3.502 \text{ \AA}, \quad L(\text{Li-Li}) = 2.67 \text{ \AA}$$

$$\text{Na} \rightarrow \quad a = 4.282 \text{ \AA}, \quad L(\text{Na-Na}) = 3.08 \text{ \AA}$$

$$\text{K} \rightarrow \quad a = 5.247 \text{ \AA}, \quad L(\text{K-K}) = 3.92 \text{ \AA}$$

$$\text{Rb} \rightarrow \quad a = 5.69 \text{ \AA}, \quad L(\text{Rb-Rb}) = 4.10 \text{ \AA}$$

$$\text{Cs} \rightarrow \quad a = 6.084 \text{ \AA}, \quad L(\text{Cs-Cs}) = 4.30 \text{ \AA}$$

Therefore, it seems logical that it is impossible to extend the covalent bond to metals. But, it's not.

If we assume that the radius of the metal is the radius of the “Bohr” orbit of the valence electron, and then calculate the half-wave length of the electron, we will see that even the allowable length of a typical “strong” covalent bond (metal) is always greater than the constant translational lattice. The de Broglie (electron) wavelength will be much larger than the lattice constant. Therefore, “weak” bonds can span several atoms (~ 3).

Further, to demonstrate what has been said, based on the Clementi radii of alkali metals [5], we calculate the wavelength and half-wave of the valence electron, and compare with the lattice constant.

Lithium:

$$\text{Li}, \quad r = 1.67 \text{ \AA}, \quad \lambda(\text{Li}) = 10.493 \text{ \AA}$$

$$a = 3.502 \text{ \AA}, \quad \lambda/2 = 5.247 \text{ \AA}.$$

Sodium:

$$\text{Na}, \quad r = 1.90 \text{ \AA}, \quad \lambda(\text{Na}) = 11.938 \text{ \AA}$$

$$a = 4.282 \text{ \AA}, \quad \lambda/2 = 5.969 \text{ \AA}.$$

Potassium:

$$\text{K}, \quad r = 2.43 \text{ \AA}, \quad \lambda(\text{K}) = 15.268 \text{ \AA}$$

$$a = 5.247 \text{ \AA}, \quad \lambda/2 = 7.634 \text{ \AA}.$$

Rubidium:

$$\text{Rb}, \quad r = 2.65 \text{ \AA}, \quad \lambda(\text{Rb}) = 16.650 \text{ \AA}$$

$$a = 5.69 \text{ \AA}, \quad \lambda/2 = 8.325 \text{ \AA}.$$

Cesium:

$$\text{Cs}, \quad r = 2.98 \text{ \AA}, \quad \lambda(\text{Rb}) = 18.724 \text{ \AA}$$

$$a = 6.084 \text{ \AA}, \quad \lambda/2 = 9.362 \text{ \AA}.$$

As you can see, the half-wavelength of the valence electron of an alkali metal is about 1.5 times longer than the lattice constant, naturally, the wavelength will be 3 times longer.

From the calculated data, it is obvious that between the nuclei of metals (metallic bond), due to the de Broglie half-wave (or wave) of valence electrons, a chemical bond can form, which is essentially similar to a covalent bond. But, since the valence electrons of the metal are socialized, the “metal covalent” bond must cover many atoms (ions). This is possible if the wavelength is increased to the required value.

Therefore, at the optimal wavelength, we will get a stable crystalline structure of the metal (the longer the wavelength, the lower the energy, but a large number of atoms are involved in the bond).

Thus, a chemical bond is a purely quantum effect that is formed between the nuclei of atoms due to de Broglie waves of valence electrons. This mechanism of bond formation can be considered universal, since from a unified theoretical standpoint it makes it possible to explain different types of chemical bonds up to intermolecular interaction.

Moreover, the physical essence of the chemical bond is simple and understandable - it is a standing wave (or half-wave) de Broglie of valence electrons between nuclei. With this approach, it is obvious that the electrons of a chemical bond are absolutely equivalent and make the same contribution to the bond.

When a chemical bond is formed from different atoms, valence electrons will have different “input” characteristics (velocity, momentum, energy, etc.), therefore, there will be a certain averaging of the characteristics of the socialized electrons that form a chemical bond.

Note. Some information about Bohr's complementarity principle.

“The principle of complementarity... formulated in 1927 by Niels Bohr. According to this principle, in order to fully describe quantum mechanical phenomena, it is necessary to apply two mutually exclusive (“additional”) sets of classical concepts, the totality of which provides comprehensive information about these phenomena as holistic.

For example, additional in quantum mechanics are space-time and energy-momentum patterns.

Descriptions of any physical object as particles and as waves complement each other, one without the other is meaningless, the corpuscular and wave aspects of the description must necessarily be included in the description of physical reality...

The principle of complementarity formed the basis of the so-called Copenhagen interpretation of quantum mechanics...

According to this interpretation, borrowed from classical physics, the dynamic characteristics of a microparticle (its coordinate, momentum, energy, etc.) are not at all inherent in the particle itself. The meaning and certain value of one or another characteristic of an electron, for example, its momentum, are revealed in connection with classical objects, for which these quantities have a certain meaning and all at the same time can have a certain value...

The role of the principle of complementarity turned out to be so significant that Wolfgang Pauli even suggested calling quantum mechanics the “theory of complementarity”, by analogy with the theory of relativity...” [10].

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